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A preliminary report on the structure of glycocyamine hemihydrate, diglycine monopicrate and 4-(N-phenyl piperizino)-6-methoxy quinaldine

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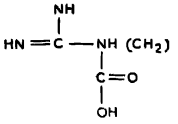
The crystal structure determination of several biologically important compounds has been undertaken in this laboratory in order to explain their functions in relation to structure. A preliminary report on the structural study of three of them is presented here.

1. *Glycocyamine hemihydrate*

Glycocyamine or guanidoacetic acid having the chemical formula



is an important amino acid. The colourless crystal grows as elongated prism on slow evaporation of an aqueous solution of the compound at room temperature.

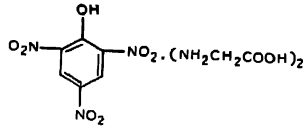
Rotation and Weissenberg X-ray photographs show that the crystal belongs to the monoclinic system with $a = 5.09$Å, $b = 6.16$Å, $c = 17.47$Å and $\beta = 95.2°$.

The only systematic absences are for $0k0$ for k odd and $h0l$ for $h+l$ odd, indicating that the space group is $P2_{1/n}$. The density of the crystal as determined by floatation method using a mixture of carbon tetrachloride and benzene has been found to be 1.526, while that calculated for 4 molecules of HN = CNHNHCH$_2$-COOH. $\frac{1}{2}$H$_2$O per unit cell is 1.525.

Complete three-dimensional data have been collected using multiple-film equiinclination Weissenberg technique with *CuKα* radiation. Intensities of the spots have been estimated by visual comparison with a calibrated strip. Spot size (Phillips 1954, 1956), Lorentz and polarization corrections have been applied to the intensity values, after which they have been brought to an absolute scale The E value or the normalized structure factor has been calculated for each of the reflections. The structure determination is in progress.

2. *Diglycine monopicrate*

The importance of the first basic amino acid glycine in living systems is well known. All amino acids form additional compounds with various acids. Leven & Van Slyke (1912) described an odd picrate of glycine, *viz.* (glycine)$_2$.picrate,

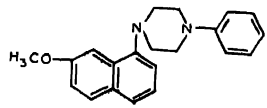


On mixing picric acid and glycine in the ratio of 1 : 1.5 by weight and freezing at 0°C, yellow tabular crystals of diglycine monopicrate are formed.

The X-ray analysis reveals that the crystal belongs to the monoclinic system. The cell constants are $a = 15.46$Å, $b = 6.92$Å, $c = 15.24$Å and $\beta = 93.2°$. The only systematic absences are $0k0$ for k odd and $h0l$ with l odd The space group is therefore $P2_{1/c}$. The observed density of the crystal is 1.55, while that calculated for 4 molecules of $C_6H_2(NO_2)_3OH(NH_2CH_2COOH)_2$ in the unit cell is 1.54. Complete three dimensional data have been collected and processed as described above. Further work on it is in progress.

3. 4-(*N-phenyl piperizino*)-6-*methoxy quinaldine*

This compound is very interesting for its medicinal properties. It is an antispasmodic agent, both neurologic and musculotropic but it has no action on uterus Its chemical formula is



and molecular weight 323. The dull light yellow coloured crystal grows as long needles on slow evaporation of a solution of the compound in methanol. The crystal is orthorhombic with $a = 8.46$Å, $b = 13\ 45$Å and $c = 16.60$Å. The observed density is 1.14, while that calculated for 4 molecules of $N_2C_{21}OH_{27}$ per unit cell is 1.13. The only systematic absences are $0kl$ for $k+1$ odd, $h0l$ for h odd, $h00$ for h odd, $0k0$ for k odd and $00l$ for l odd, indicating the space group to be either $Pna2_1$ or $P2_{1/n}2_{1/a}2_{1/m}$. The latter space group requires 8 molecules per unit cell, and to accommodate only 4 the molecule must have a mirror or 2-fold symmetry which is extremely unlikely in this case. The space group is therefore most probably $Pna2_1$. For this crystal also the three dimensional intensity data have been collected and processed. The structure determination is in progress.

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